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A New Method to Evaluate the Similarity of Chromatographic Fingerprints: Weighted Pearson Product–Moment Correlation Coefficient

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Abstract

The Pearson product–moment correlation coefficient is being used to evaluate the similarity of the high-performance liquid chromatographic fingerprints of traditional Chinese medicine (TCM) in China. It is confirmed that a large range of peak areas produced the wrong results. A new algorithm concerning weighted Pearson product–moment correlation coefficient is proposed in this article. The results for both real cases and simulated data sets show that the weighted Pearson product–moment correlation coefficients allow relatively larger differences for large values, smaller differences for small values, and more reliable results than the unweighted Pearson product–moment correlation coefficients. Weight selection depends on the specific scientific problem.

Introduction

Traditional Chinese medicine (TCM) has been used in China for thousands of years, and its curative effect has been certified. But quality control is one of the most difficult problems. A fingerprinting technique is prescribed to control the quality of the injections of TCM. The content of TCM components can be reflected by the peaks areas of the chromatographic fingerprint. The stable area of the peaks is a pre requisite to stable quality of TCM. The similarity measures can reflect the differences of the peak areas of two chromatographic fingerprints.

The Pearson product–moment correlation coefficient is one of the association measures (1). It was introduced by Karl Pearson (2) and has been used to evaluate the similarity of spectrum, electrophoresis, and other kinds of data sets (3–6).

The Pearson product–moment correlation coefficient r for variables x and y is described as follows (7):

$$r = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2 \sum_{i=1}^{n}(y_i - \bar{y})^2}} \quad \text{Eq. 1}$$

where $\bar{x}$ and $\bar{y}$ are the averages of the x and y measurements and donates summation over all n observations.

This correlation coefficient is widely applied to evaluate the similarity of the chromatographic fingerprints of TCM (8,9) in China. Some studies have found those that are not sensitive to proportional or additive changes as a similarity measure (10). If the range of the data is wide, the Pearson product–moment correlation coefficient often seems close to 1 (10,13). Both normalizing transformation and logarithmic transformation of data sets have been used before calculating the Pearson product–moment correlation coefficient (12,13). In this article, a new algorithm named the weighted Pearson product–moment correlation coefficient is proposed. It can allow relatively larger differences for large values and smaller differences for small values. The results show it is able to deal with some cases meeting the mentioned problems. And more reliable results than the unweighted Pearson product–moment correlation coefficients were obtained for both real cases and simulated data sets.

Theory

The Pearson product–moment correlation coefficient r can be deduced from the slope b and intercept a of the simple regression line of y on x (14). For the simple regression line $y = a + bx$:

$$b = l_{xy}/l_{xx} \ , \ a = \bar{y} - b\bar{x} \quad \text{Eq. 2}$$

Among which

$$l_{xy} = \sum_{i=1}^{n}\left(x_i - \bar{x}\right)\left(y_i - \bar{y}\right) \quad \text{Eq. 3}$$

and

$$l_{xx} = \sum_{i=1}^{n}\left(x_i - \bar{x}\right)^2 \ , \ l_{yy} = \sum_{i=1}^{n}\left(y_i - \bar{y}\right)^2 \quad \text{Eq. 4}$$

The Pearson product–moment correlation coefficient r is calculated according to the formula:

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$$r = l_{xy} \Big/ \sqrt{l_{xx} l_{yy}} \quad \text{Eq. 5}$$

We introduced the weighted Pearson product–moment correlation coefficient r from the slope b and intercept a of the weighted regression line of y on x where:

$$l_{xy} = \sum_{i=1}^{n} w_i \left(x_i - \bar{x}\right)\left(y_i - \bar{y}\right) \quad \text{Eq. 6}$$

and:

$$l_{xx} = \sum_{i=1}^{n} w_i \left(x_i - \bar{x}\right)^2 , \quad l_{yy} = \sum_{i=1}^{n} w_i \left(y_i - \bar{y}\right)^2 \quad \text{Eq. 7}$$

Therefore, the weighted Pearson product–moment correlation coefficient r_w can be calculated according to the formula:

$$r_w = \frac{\sum_{i=1}^{n} w_i (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n} w_i (x_i - \bar{x})^2 \sum_{i=1}^{n} w_i (y_i - \bar{y})^2}} \quad \text{Eq. 8}$$

Among which:

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} w_i x_i \qquad \bar{y} = \frac{1}{n}\sum_{i=1}^{n} w_i y_i \quad \text{Eq. 9}$$

For the weighted regression line, the usual weights are as $w_i = k/x_i$ or $w = k/x_i^2$. Because there are no dependent variables or independent variables in the comparison of similarity, we combined $1/x$ and $1/y$ together as a weighting factor:

$$w_1 = \frac{1}{2}\left(\frac{1}{x_i} + \frac{1}{y_i}\right) = \frac{x_i + y_i}{2x_i y_i} \quad \text{Eq. 10}$$

as well as $1/x^2$ and $1/y^2$ as another weighting factor:

$$w_2 = \frac{1}{2}\left(\frac{1}{x_i^2} + \frac{1}{y_i^2}\right) = \frac{x_i^2 + y_i^2}{2x_i^2 y_i^2} \quad \text{Eq. 11}$$

Experimental

The Yinzhihuang injection is composed of baicalin and the extractions of *Cardenia jasminoides Ellis, Artemisia Capillris Thunb*, and *Lonicera japonica.* This is used in China as a cure for hepatitis. A reversed-phase high-performance liquid chromatographic (HPLC) method was developed to analyze Yinzhihuang injections. A Shimadzu LC-10AT HPLC was used (Kyoto, Japan). A Shimadzu SPD-10A UV detector was set at a wavelength of 230 nm. A mobile phase of methanol–sodium dihydrogen phosphate (0.1 mol/L, pH 2.5)–tetrahydrofuran (40:80:16) was delivered at a flow rate of 1 mL/min. Twenty microliters of solution was analyzed on the C_{18} column (20 cm × 4.6 mm, 5 µm) (Dalian Elite Scientific Instruments Co., Dalian, China). The analysis was carried out at 30°C.

Yinzhihuang injections were manufactured by Jiangsu Wujin Pharmaceutical Factory (Jiangsu, China). The reference materials (baicalin, gardenoside, and chlorogenic acid) were purchased from the National Institute for the Control of Pharmaceutical and Biological Products (Beijing, China).

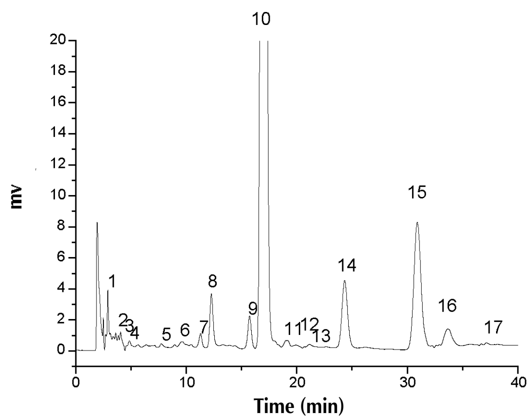

Figure 1. The HPLC chromatogram of Yinzhihuang Injection and the 17 common peaks.

Table I. The Relative Areas of the Common Peaks in the 10 Samples of Yinzhihuang Injection

Peak	1	2	3	4	5	6	7	8	9	10	RSD (%)
1	6.424	6.522	6.636	6.705	6.438	6.176	6.105	6.113	6.413	6.343	3.3
2	4.045	3.987	4.085	4.201	5.514	4.407	3.827	4.286	3.806	4.116	11.6
3	1.608	1.592	1.429	1.381	1.588	1.363	1.038	1.921	1.057	1.240	19.1
4	1.499	1.357	1.004	1.446	1.409	0.9645	1.201	1.079	2.152	1.308	25.4
5	1.647	1.617	2.129	1.208	1.616	2.063	1.984	3.432	1.286	2.143	33.0
6	1.846	1.764	2.144	2.244	1.816	2.412	2.012	2.305	1.673	2.008	12.4
7	4.151	4.177	4.186	4.825	4.044	4.223	4.413	3.047	2.811	3.436	16.1
8	19.64	19.50	19.46	18.93	21.33	18.87	19.61	20.72	21.02	21.46	4.9
9	12.72	12.57	12.53	12.56	12.62	12.08	11.70	7.950	12.16	13.68	12.8
10	1417.1	1493.9	1343.7	1334.9	1388.5	1318.3	1567.7	1527.1	1395.4	1350.9	6.2
11	3.300	2.715	3.051	3.118	3.311	2.984	2.838	2.627	4.035	3.102	12.8
12	1.639	1.666	1.236	2.260	1.682	1.209	1.375	1.744	1.679	1.613	18.7
13	1.300	1.618	1.601	1.262	1.102	0.7584	1.512	1.176	1.811	2.400	31.0
14	39.70	43.03	40.65	41.35	39.77	40.40	43.07	46.63	39.86	43.42	5.4
15	100	100	100	100	100	100	100	100	100	100	0
16	13.62	13.76	14.18	15.56	13.56	14.73	13.98	14.98	14.66	13.63	4.8
17	0.9270	0.9034	0.9493	0.9230	0.9538	0.9292	1.2612	0.8320	0.9466	1.0496	12.0

Table II. The Pearson Product–Moment Correlation Coefficients According to the Changes of y_1 and y_{100}

Changes of y_1	Relative changes (%)	Correlation coefficients	Changes of y_{100}	Relative changes (%)	Correlation coefficients
1	0	1	100	0	1
2	100	0.999994	101	1	0.999994
3	200	0.99998	102	2	0.99998
4	300	0.99994	103	3	0.99995
5	400	0.99991	104	4	0.99991
6	500	0.9999	105	5	0.9999
7	600	0.9996	106	6	0.9998

Sample preparation

One milliliter of the Yinzhihuang injection was diluted to 50 mL with methanol and filtered through a 0.45-µm membrane prior to analysis. The data sets were calculated by Matlab 5.3 (the MathWorks, Inc., Natick, MA).

Results and Discussion

The HPLC signals were collected until all of the components were eluted from the column. After comparing chromatograms of the 10 samples of Yinzhihuang injections, 17 common peaks were found (the 17 common peaks are marked in Figure 1).

Table III. The Pearson Product–Moment Correlation Coefficients after the Peaks No. 10 Were Reduced to 1%

	1	2	3	4	5	6	7	8	9	10
1	1.0000									
2	0.9995	1.0000								
3	0.9999	0.9996	1.0000							
4	0.9996	0.9995	0.9997	1.0000						
5	0.9997	0.9991	0.9996	0.9992	1.0000					
6	0.9997	0.9994	0.9999	0.9998	0.9995	1.0000				
7	0.9993	0.9999	0.9994	0.9993	0.9989	0.9993	1.0000			
8	0.9962	0.9979	0.9969	0.9969	0.9962	0.9969	0.9983	1.0000		
9	0.9996	0.9991	0.9995	0.9993	0.9996	0.9993	0.9989	0.9964	1.0000	
10	0.9991	0.9996	0.9994	0.9990	0.9991	0.9990	0.9993	0.9974	0.9991	1.0000

Table IV. The Weighted Pearson Product–Moment Correlation Coefficients of the 10 Samples of the Yinzhihuang Injection*

Samples	Weight	1	2	3	4	5	6	7	8	9	10
1	w_1	1.0000									
	w_2	1.0000									
2	w_1	0.9998	1.0000								
	w_2	0.9958	1.0000								
3	w_1	0.9997	0.9993	1.0000							
	w_2	0.9843	0.9869	1.0000							
4	w_1	0.9995	0.9990	0.9996	1.0000						
	w_2	0.9879	0.9848	0.9612	1.0000						
5	w_1	0.9998	0.9994	0.9996	0.9995	1.0000					
	w_2	0.9947	0.9874	0.9774	0.9844	1.0000					
6	w_1	0.9995	0.9990	0.9998	0.9996	0.9995	1.0000				
	w_2	0.9729	0.9584	0.9735	0.9550	0.9781	1.0000				
7	w_1	0.9994	0.9998	0.9987	0.9982	0.9988	0.9983	1.0000			
	w_2	0.9807	0.9828	0.9885	0.9666	0.9734	0.9675	1.0000			
8	w_1	0.9983	0.9987	0.9981	0.9973	0.9980	0.9979	0.9989	1.0000		
	w_2	0.9505	0.9495	0.9630	0.9078	0.9483	0.9600	0.9461	1.0000		
9	w_1	0.9996	0.9993	0.9993	0.9992	0.9994	0.9989	0.9987	0.9978	1.0000	
	w_2	0.9724	0.9683	0.9412	0.9633	0.9613	0.9016	0.9560	0.8868	1.0000	
10	w_1	0.9993	0.9990	0.9997	0.9993	0.9994	0.9992	0.9983	0.9976	0.9994	1.0000
	w_2	0.9755	0.9847	0.9862	0.9566	0.9606	0.9166	0.9840	0.9432	0.9694	1.0000

* $w_1 = \frac{x+y}{2xy}$, $w_2 = \frac{x^2+y^2}{2x^2y^2}$.

Peak 15 is used as the internal standard. The other areas are the relative areas. The relative areas of the 17 common peaks of the 10 samples of the Yinzhihuang injection are shown in Table I.

The similarity of the 10 samples can be evaluated with the Pearson product–moment correlation coefficient. After calculating all the Pearson product–moment correlation coefficients between any two of the 10 samples, it was observed that all were located between 0.9999 and 1.0000, which means the 10 samples had great similarity. But an examination of the data in Table I reveals that this was not the case. They did have some clear differences. As the larger of the relative standard deviations (%), the difference should have been greater. The results show that the Pearson product–moment correlation coefficient was not sensitive to the signal differences of the samples.

Deficiencies of the Pearson product–moment correlation coefficient

In order to study the deficiencies of the Pearson product–moment correlation coefficient, we designed and tested some simple but persuasive examples.

Example 1

To two variables, x (1, 2, 3,…100) and y (1, 2, 3,…100), we made some changes in the first (y_1) and last number (y_{100}) of y, respectively (y_1 was changed from 1 to 7 and y_{100} was changed from 100 to 106). The Pearson product–moment correlation coefficients between x and y were then calculated (Table II).

From Table II, we can see that the Pearson product–moment correlation coefficients turned out little difference when y_1 and y_{100} changed with the same absolute quantities. The similarity was not identical when the same absolute differences occured on the small or the large values. However, the Pearson product–moment correlation coefficient cannot reflect the different relative changes caused by the same absolute changes.

Example 2

The Pearson product–moment correlation coefficients between any two of the 10 Yinzhihuang injections were between 0.9999 and 1.0000. Here we have the peak no. 10 of all of the 10 samples reduced to its 1%. That means the relative differences of the samples did not change, but the absolute differences decreased greatly. The Pearson product–moment correlation coefficients were then calculated. The results are shown in the Table III.

These results show that all of the Pearson product–moment correlation coefficients between any two of the 10 samples decreased, to some extent. Does this mean the similarities decreased after the change? This was certainly not the case. It was concluded that the Pearson product–moment correlation coefficient was affected by the signal range of the samples (7,11).

The weighted Pearson product–moment correlation coefficient

Now we used the weighted Pearson product–moment correlation coefficient to evaluate the similarity of the 17 common peaks of the 10 samples of the Yinzhihuang injection. The results are given in the Table IV.

From these results we can see that the weighted Pearson product–moment correlation coefficient decreased and performed well. The sensitivity of the weighted correlation coefficient was greater than original correlation coefficient. The differences of the 10 samples can be clearly shown out.

In example 1, the Pearson product–moment correlation coefficient cannot reflect the relative differences caused by the same absolute differences. Now we used the weighted Pearson product–moment correlation coefficient to evaluate the similarity. The results are shown in Table V.

From these results we can see that the weighted Pearson product–moment correlation coefficient can reflect the different relative differences caused by the same absolute differences. When the absolute differences were equal the similarity decreases with the increase of the relative differences.

Table V. The Weighted Pearson Product–Moment Correlation Coefficients*

Changes of y_1	Correlation coefficients w_1	w_2	Changes of y_{100}	Correlation coefficients w_1	w_2
1	1	1	100	1	1
2	0.99992	0.9970	101	0.999999	0.9999995
3	0.9997	0.9894	102	0.999996	0.999998
4	0.9994	0.9777	103	0.999991	0.999996
5	0.9990	0.9624	104	0.99998	0.999992
6	0.9985	0.9441	105	0.99998	0.99999
7	0.9979	0.9234	106	0.99996	0.99998

* According to the changes of y_1 and y_{100}, $w_1 = \frac{x+y}{2xy}$, $w_2 = \frac{x^2+y^2}{2x^2y^2}$.

Table VI. The Pearson Product–Moment Correlation Coefficients after Logarithmic Transformation for Example 1

Changes of y_1	Correlation coefficients e	10	Changes of y_{100}	Correlation coefficients e	10
1	1	1	100	1	1
2	0.9975	0.9975	101	0.9999994	0.9999994
3	0.9936	0.9936	102	0.999998	0.999998
4	0.9895	0.9895	103	0.999995	0.999995
5	0.9857	0.9857	104	0.999991	0.999991
6	0.9821	0.9821	105	0.99999	0.99999
7	0.9787	0.9787	106	0.99998	0.99998

Comparison between the weighted Pearson product–moment correlation coefficient and using normalizing transformation and logarithmic transformation

A possible way to solve such a problem is to perform a pretreatment for the original data sets. Both normalizing transformation and logarithmic transformation have been applied before calculating the Pearson product–moment correlation coefficient (12,13). After transformation, the Pearson product–moment correlation coefficient was calculated.

In case of the normalizing transformation, the Pearson product–moment correlation coefficients between any two of the 10 Yinzhihuang injections were still between 0.9999 and 1.0000.

The Pearson product–moment correlation coefficients after logarithmic transformation have also been calculated for example 1. The results are shown in Table VI. After normalizing the transformation and logarithmic transformation, the range of the data decreases greatly. But the Pearson product–moment correlation coefficients nearly did not change after normalization. The Pearson product–moment correlation coefficient r is computed as follows after normalization:

$$r = \frac{\sum_{i=1}^{n}\left(\frac{x_i}{\sum_{i=1}^{n} x_i} - \frac{\bar{x}}{\sum_{i=1}^{n} x_i}\right)\left(\frac{y_i}{\sum_{i=1}^{n} y_i} - \frac{\bar{y}}{\sum_{i=1}^{n} y_i}\right)}{\sqrt{\sum_{i=1}^{n}\left(\frac{x_i}{\sum_{i=1}^{n} x_i} - \frac{\bar{x}}{\sum_{i=1}^{n} x_i}\right)^2 \sum_{i=1}^{n}\left(\frac{y_i}{\sum_{i=1}^{n} y_i} - \frac{\bar{y}}{\sum_{i=1}^{n} y_i}\right)^2}} = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2 \sum_{i=1}^{n}(y_i - \bar{y})^2}} \quad \text{Eq. 12}$$

From this equation, the normalization factor in the numerator and the denominator appears to cancel each other, and the final form is simply the standard equation for r. The purpose of normalization is to identify and remove systematic variation. But it cannot improve the sensitivity of the Pearson product–moment correlation coefficient.

After logarithmic transformation, the Pearson product–moment correlation coefficients changed a lot because of the changes of the differences (Figure 2). In this case, the point of tangency of $y = \ln(x)$ and $y = x - 1$ is (1,0). The slope of the tangent of $y = \ln(x)$ was less than 1 when $x > 1$, and the slope of the tangent of $y = \ln(x)$ was larger than 1 when $x < 1$. The slope of the tangent showed the speed of the changes of y against x. That is to say the absolute differences decreased after the log(e) – transformation when $x > 1$ and that the absolute differences increased after the log(e) – transformation when $x < 1$. The relative differences of the small values changed much more than the large values.

By comparing the Pearson product–moment correlation coefficients after logarithmic transformation with weighted coefficients, we can see that the similarity all decreased, to some extent. But they were certainly not the same thing. As for the logarithmic transformation, the differences of the large values were decreased, and those of the small values were relatively increased. It confirmed that the characters of the data had changed. The results after logarithmic transformation are shown in Table VII.

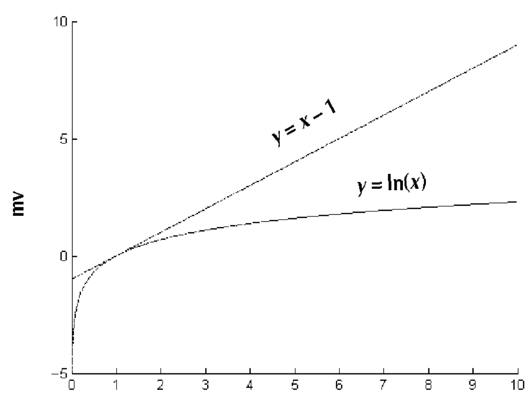

Figure 2. The change-curve of variables after log(e)-transformation.

Table VII. The Data Sets of the 10 Samples of Yinzhihuang Injection after log(e) – Transformation

Peak	1	2	3	4	5	6	7	8	9	10	RSD (%)
1	1.8600	1.8752	1.8925	1.9029	1.8622	1.8207	1.8091	1.8104	1.8583	1.8474	1.8
2	1.3975	1.3830	1.4073	1.4353	1.7073	1.4832	1.3421	1.4554	1.3366	1.4149	7.4
3	0.4750	0.4650	0.3570	0.3228	0.4625	0.3097	0.0373	0.6528	0.0554	0.2151	57.7
4	0.4048	0.3053	0.0040	0.3688	0.3429	–0.0361	0.1832	0.0760	0.7664	0.2685	87.0
5	0.4990	0.4806	0.7557	0.1890	0.4800	0.7242	0.6851	1.2331	0.2515	0.7622	49.3
6	0.6130	0.5676	0.7627	0.8083	0.5966	0.8805	0.6991	0.8351	0.5146	0.6971	17.7
7	1.4233	1.4296	1.4317	1.5738	1.3972	1.4405	1.4846	1.1142	1.0335	1.2343	12.7
8	2.9776	2.9704	2.9684	2.9407	3.0601	2.9376	2.9760	3.0311	3.0455	3.0662	1.7
9	2.5432	2.5313	2.5281	2.5305	2.5353	2.4916	2.4596	2.0732	2.4983	2.6159	6.0
10	7.2564	7.3091	7.2032	7.1966	7.2360	7.1841	7.3574	7.3311	7.2409	7.2085	0.9
11	1.1939	0.9988	1.1155	1.1372	1.1973	1.0933	1.0431	0.9658	1.3950	1.1320	10.8
12	0.4941	0.5104	0.2119	0.8154	0.5200	0.1898	0.3185	0.5562	0.5182	0.4781	39.7
13	0.2624	0.4812	0.4706	0.2327	0.0971	–0.2765	0.4134	0.1621	0.5939	0.8755	94.5
14	3.6814	3.7619	3.7050	3.7221	3.6831	3.6988	3.7628	3.8422	3.6854	3.7709	1.4
15	4.6052	4.6052	4.6052	4.6052	4.6052	4.6052	4.6052	4.6052	4.6052	4.6052	0
16	2.6115	2.6218	2.6518	2.7447	2.6071	2.6899	2.6376	2.7067	2.6851	2.6123	1.8
17	–0.0758	–0.1016	–0.0520	–0.0801	–0.0473	–0.0734	0.2321	–0.1839	–0.0549	0.0484	–285.6

For the weighted Pearson product–moment correlation coefficient, the characters of the data did not change at all. Its improved sensitivity can be explained from the weighted regression line. For the simple regression line, there are no large derivations from the line for all of the values. But for the weighted regression line, large values can have relatively larger derivation, and small values can have relatively smaller derivation. The same absolute difference on the small values or on the large values has almost the same effect on the Pearson product–moment correlation coefficient. Using the weighted Pearson product–moment correlation coefficient, the similarity will decrease when the same absolute difference on the small values than on the large values.

Conclusion

From the preceeding, the conclusion can be made that weighted Pearson product–moment correlation coefficient is necessary when the range of the peak areas is large. The characters of the data do not change. It allows relatively larger differences for large values and smaller differences for small values. The results are more reliable than the Pearson product–moment correlation coefficients. The selection of the weight depends on the specific scientific cases.

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